2-Hydroxy-3-methoxybenzaldehyde 148-53-8 | DTXSID5022011

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	1.14	0.85	1.12	0.83	1.23	

Model Results

Predicted value: 3.12e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.47e-01

Confidence level: 6.91e-01

Nearest Neighbors from the Training Set

Image not found

2-Methyl-p-benzoquinone Measured: 2.35e-11 Predicted: 2.15e-11

Image not found

1,4-Benzoquinone Measured: 4.60e-12 Predicted: 5.97e-12